

Fermi-pocket-vanishing phase transition in the ferromagnetic phase of the Kondo lattice model

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By performing extensive dynamical mean-field theory calculations with the numerical renormalization group as the impurity solver, we establish the low-temperature phase diagrams of the spin-1/2 and spin-1 Kondo lattice models as a function of the conduction-band filling and the exchange coupling strength in the regime of ferromagnetic RKKY interactions (i.e., for low and moderate electron density). We show that *both* models have *two* distinct ferromagnetic phases separated by a continuous Lifshitz transition of the Fermi pocket vanishing type: one phase has a true gap in the minority band, the other only a pseudogap. The two phases can be experimentally distinguished by their magnetization curves; only the first phase exhibits magnetization rigidity. We find that, quite generically, ferromagnetism and Kondo screening coexist rather than compete, both in spin-1/2 and spin-1 models. We compute the Curie temperatures and establish a “ferromagnetic Doniach diagram” for both models.

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Materials with competing interactions have complex low-temperature phase diagrams with quantum phase transitions separating the different ground states [1–3]. Heavy-fermion compounds containing ions with partially filled f shells show a particularly wide range of ordered phases [3–6]. The paradigmatic model for these materials is the Kondo lattice model (KLM) [7–9] which describes a conduction band of itinerant non-interacting electrons and a lattice of local moments; the itinerant and localized electrons are coupled at each site by an antiferromagnetic exchange interaction J . For large J , the itinerant electrons screen the local moments in a lattice version of the Kondo effect. The resulting state is paramagnetic with Fermi liquid properties, albeit with strongly renormalized parameters. For small J , however, the conduction-band electrons behave as carriers of the long-range RKKY interaction which leads to magnetic ordering of the local moments. The two regimes are separated by a quantum phase transition at critical J^* . This competition between the local Kondo effect and the intersite exchange interaction is described by the Doniach diagram [10]. While the Kondo temperature is an exponentially increasing function of J , $T_K \propto \exp(-1/\rho J)$, the Néel temperature increases at first quadratically with J , but then it peaks and decreases to zero at J^* as the strong Kondo screening takes over. The simplest version of the KLM with spin-1/2 local moments indeed has an antiferromagnetic (AFM) ground state (Néel order) for small J near half-filling of the conduction band [11, 12]. The nature of the quantum phase transition at the critical J^* has been investigated using a variety of methods, the most accurate of which confirm that the transition is second order (quantum critical) and indicate that it involves a change of the Fermi surface topology [13–15]. In the spin-1 KLM, there is no phase transition at half-filling and the AFM phase extends to large values of J .

While cerium compounds commonly have antiferromagnetic ground state, some are ferromagnetic (FM): CeRu_2Ge_2 [16], CeIn_2 [17, 18], and $\text{CeRu}_2\text{Al}_2\text{B}$ [19]. A number of uranium and neptunium heavy-fermion materials are also FM:

UTe [20], $\text{UCu}_{0.9}\text{Sb}_2$ [21], $\text{UCo}_{0.5}\text{Sb}_2$ [22], NpNiSi_2 [23], Np_2PdGa_3 [24], and UCu_2Si_2 [25]. In addition, there are strong indications of robust coexistence of the Kondo effect and ferromagnetism, in particular in U compounds. In Refs. [25–29] it has been proposed that an appropriate minimal model for this behavior is the spin-1 version of the KLM, where the conduction-band electrons underscreen the local moments, while the residual moments order ferromagnetically. FM order appears for low and moderate electron filling in the conduction band [26, 30–33]. Mean-field analysis predicts two phases: for small J the stable phase is a FM regular metal (i.e., the hybridization mean-fields are zero, while the magnetization mean-fields are finite), while for large J there is a transition to a FM heavy metal (i.e., both mean-fields are non-zero). Dynamical mean-field theory (DMFT) calculations demonstrated that the standard spin-1/2 KLM also has a FM order coexisting with (incomplete) Kondo screening [34]. Furthermore, this phase turned out to be a half-metal (the minority spin band is gapped [35]) and there is a commensurability condition relating the magnetization to the band filling [34], which can be interpreted within the hybridization mean-field picture as being due to completely filled minority-spin lower band [36, 37]. A recent mean-field analysis of the spin-1/2 model suggested the presence of several different ferromagnetic phases [38]. So far, however, a single FM phase has been identified in the DMFT calculations [32, 33].

These findings open a number of important questions: What is the relationship between ferromagnetism and Kondo screening: do they compete or coexist? If there is some degree of competition, how does it manifest? What is the minimal model for studying these effects, spin-1/2 or spin-1 KLM? Is there a quantum phase transition between different FM states also in the spin-1/2 model? What is the nature of these transitions and what are their experimental signatures? And, finally, which aspects of the static mean-field analysis are correct and which must be revised in more accurate dynamical treatment? To answer these questions we have performed extensive DMFT [39] calculations using the numerical renor-

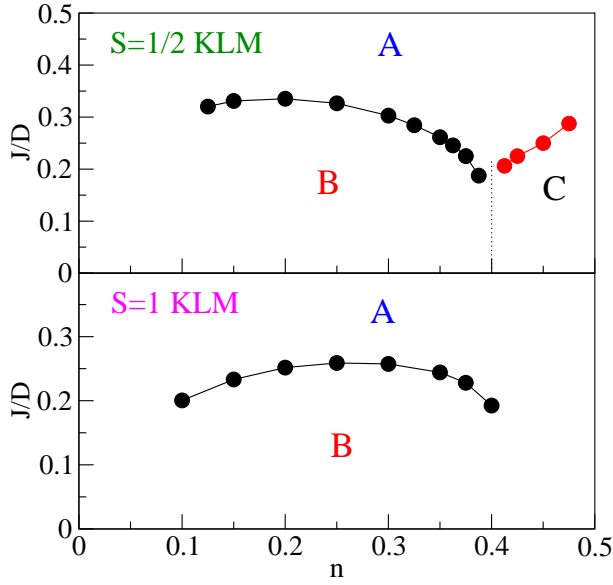


Figure 1: (Color online) Phase diagrams of spin-1/2 and spin-1 Kondo lattice models for small and intermediate occupancies n . Phase A is a ferromagnetic half-metal phase with strong Kondo effect where the minority band is gapped. Phase B is an itinerant ferromagnetic phase with a pseudogap. Phase C for spin-1/2 model indicates the region where the true ground state is expected to be a charge density wave. For very small occupancies, the calculations fail to converge due to limitations of the impurity solver.

malization group (NRG) as the impurity solver [40–45].

We consider the Kondo lattice model

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} (\epsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + J \sum_i \mathbf{s}_i \cdot \mathbf{S}_i, \quad (1)$$

which describes a single-orbital conduction band with dispersion $\omega = \epsilon_{\mathbf{k}}$, and a lattice of local moments described by the spin- S operators \mathbf{S}_i ; \mathbf{s}_i is the conduction-band spin-density at site i , and J is the antiferromagnetic Kondo exchange coupling ($J > 0$). We focus on the Bethe lattice that has a semi-circular density of states with bandwidth $2D$.

In Fig. 1 we present the main result of this work: the phase diagrams of the spin-1/2 and spin-1 KLM as a function of the band filling, $n < 0.5$, and the strength of the exchange coupling, J . For both spins, 1/2 and 1 alike, we find two different ferromagnetic phases. The one at large J (phase A) corresponds to the ferromagnetic half-metal phase described by Peters et al. [34]. The corresponding spin-resolved spectral functions for the $S = 1$ model are shown in Fig. 2, panel A. The minority spin band is gapped [34], while the majority band only exhibits a weak hybridization pseudo-gap characteristic of the Kondo lattice systems [46, 47]. The phase at small J (phase B) is not gapped, but there is a pronounced pseudogap just below the Fermi level in the minority band, Fig. 2, panel B. The spectral functions for the $S = 1/2$ model are qualitatively the same. The spectra thus suggest the occurrence of a Lifshitz transition: there is no change in the symmetry, but the Fermi surface of the minority band shrinks to

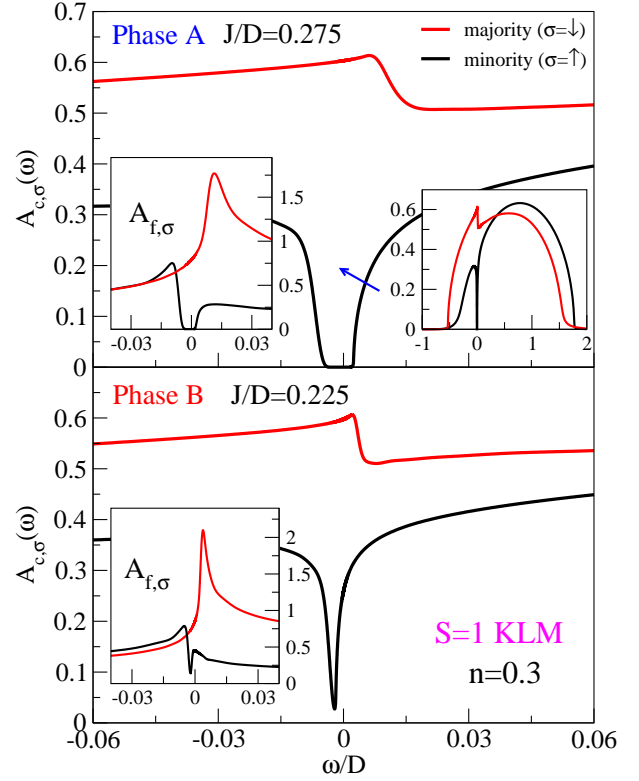


Figure 2: (Color online) Spin-resolved conduction-band local spectral functions $A_{c,\sigma}$ for the spin-1 KLM in the ferromagnetic half-metal phase (A) and in the itinerant ferromagnetic phase (B). The arrow indicates the main effect of decreasing interaction J : the lower edge of the upper hybridized band shifts to lower frequencies. The left insets in both panels show the f -level spectral functions $A_{f,\sigma}$ defined through the imaginary part of the scattering T matrix. The right inset in the upper panel shows the spectral functions in the full frequency interval.

a point and disappears as one goes from phase B to A. We emphasize that the two phases exist both for spin-1/2 and for spin-1 models and have similar properties; clearly, the *value of the spin does not play a crucial role in the FM ordering*.

The transition point J^* is a non-monotonic function of filling that peaks at $n \sim 0.2$ and $n \sim 0.25$, respectively. Near $n \sim 0.4$ we observe a change of behavior in the small- J phase. For $S = 1/2$ KLM, this is the parameter regime where a charge-density wave (CDW) ground state is predicted [33], but not allowed for in our calculations.

In order to study the nature of the phase transition between A and B more carefully, we plot in Fig. 3 the evolution of the magnetization (both total, and for the conduction-band c and localized f electrons separately) and of the quasiparticle renormalization factors

$$Z_\sigma = \left[1 - \frac{\partial}{\partial \omega} \Sigma_\sigma(\omega) \Big|_{\omega=\mu} \right]^{-1} \quad (2)$$

as a function J across the transition point J^* . The frozen magnetization in phase A is given by a generalization of the

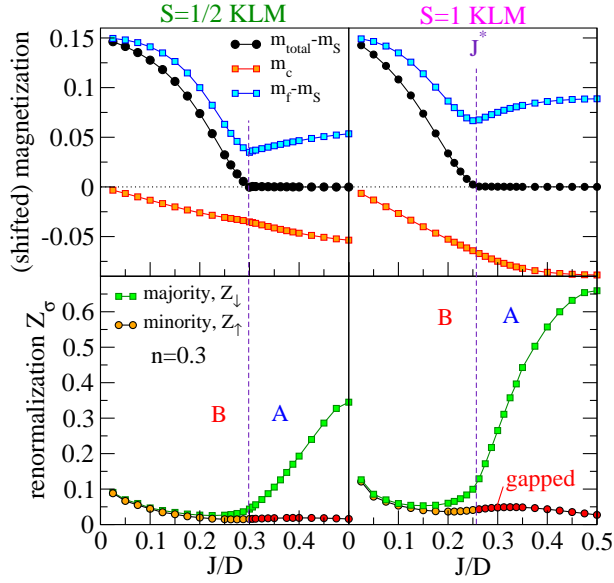


Figure 3: (Color online) Total, conduction-band c -level and localized f -level magnetizations (top panels) and the spin-dependent quasiparticle renormalization factors Z_σ (bottom panels) across the phase transition, indicated by the vertical dashed lines. The magnetization is here defined as the expectation value of the spin operator without the $-g\mu_B$ factor: $m_f = \langle S_z \rangle$, $m_c = (n_\uparrow - n_\downarrow)/2$, $m_{\text{total}} = m_f + m_c$. In the plots, m_{total} and m_f are shifted by m_S defined in Eq. (3).

spin-1/2 KLM result from Refs. [34, 36, 37]:

$$m_S = (2S - n)/2. \quad (3)$$

The magnetization is continuous, but there is a change of slope in m_f , while m_c has a continuous first derivative. This is in disagreement with the static mean-field analysis for $S = 1$, which predicts a large jump in the magnetization [27]. The renormalization factors Z_σ for both spin orientations are continuous and finite across the transition (note that in the minority band of phase A there are no quasiparticles, but Z_σ can formally still be defined). There is no criticality in this spin selective metal-insulator transition. From these results we may conclude that this is a *continuous Lifshitz transition of the Fermi pocket vanishing type* [36, 37, 48–51]. The change of the Fermi surface topology is continuous in the sense that there is no sudden reorganization of the Fermi surface. Deep in the phase A, the majority electrons become weakly correlated (Z saturates at a value of order 0.5).

For very large J , there is another Lifshitz transition to a non-gapped phase [52] that we denote as B'. While in the BA transition, the chemical potential is located at the *bottom of the upper hybridized band*, in the AB' transition the chemical potential is located at the *top of the lower hybridized band* at the transition point. In other words, while BA corresponds to the vanishing of electron pocket, AB' corresponds to the emergence of hole pocket. The AB' transition occurs at unphysically large values of J in excess of the bandwidth (the Schrieffer-Wolff transformation mapping the periodic Ander-

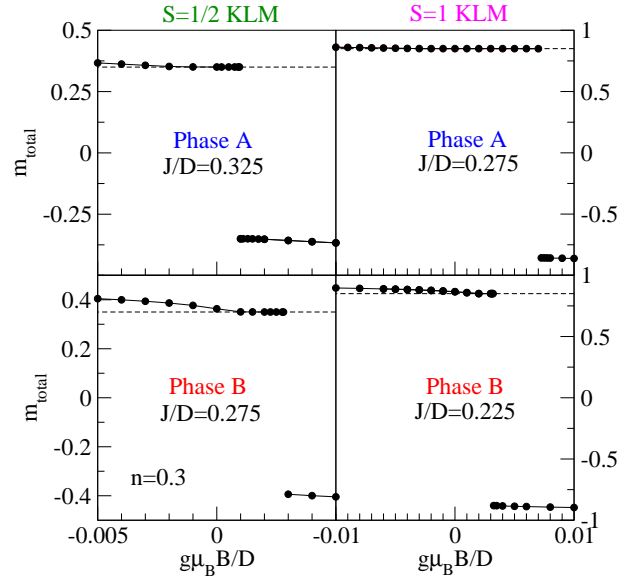


Figure 4: (Color online) Magnetization in longitudinal external magnetic field. The dashed lines indicate the value of the frozen magnetization m_S . The g -factors are assumed equal for c and f levels, $g_c = g_f = g$.

son model to the KLM ceases to be valid), therefore we do not plot them in the phase diagram. For spin-1/2 model with $n = 0.3$, this AB' transition occurs at $J/D = 2.25$. For even larger J , the system eventually becomes paramagnetic in the ground state. For $n = 0.3$, this occurs for $J/D = 3.4$.

The static mean-field also predicts four distinct phases at $T = 0$ [38]: ferromagnetic, "spin-polarized" Kondo, "spin-non-polarized" Kondo, and paramagnetic phase, the first three roughly corresponding to our B, A, and B'. We find, however, that all four phases that we find exhibit the Kondo effect, i.e., our phase B is not pure ferromagnetic. Furthermore, the Lifshitz transitions we find are all continuous: there are no jumps in any of our results. Finally, we note that the DMFT predicts that deep inside B and B' phases there are pseudo-gaps rather than gaps (this is due to non-zero imaginary part of the self-energy, i.e., due to correlation effects). The most surprising outcome of the DMFT calculations is, therefore, the gradual emergence of true gaps from pseudo-gaps as the gapped phase A is approached from B or from B', while the mean-field results are closer to the rigid-band picture.

Does the existence of multiple phases indicate a competition between the RKKY interaction and the Kondo effect? Some degree of antagonism is suggested by the fact that the f -shell magnetization m_f has a minimum at the BA Lifshitz point where both tendencies are expected to be equally strong and, furthermore, it could be argued that m_f increases with J in phase A only because Kondo screening is rendered incomplete by the opening and widening of the gap. Nevertheless, this competition does not imply mutual exclusion and most results rather support the notion of robust coexistence.

Experimentally the phases A and B can be distinguished

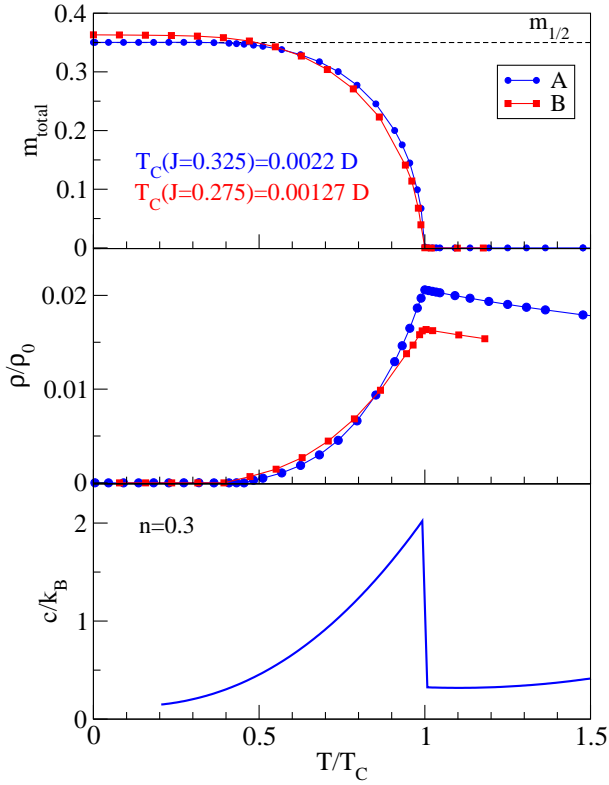


Figure 5: (Color online) Temperature dependence of the magnetization, resistivity and heat capacity for the spin-1/2 Kondo lattice model in phases A and B. The horizontal axis is rescaled by the Curie temperature T_C . Resistivity is in units of $\rho_0 = 2\pi e^2 \Phi(0)/\hbar D$, where Φ is the transport integral. Heat capacity curve was obtained by differentiating a piecewise interpolation of the numerical results for the total energy.

by their magnetization curves. In phase A, m_{total} remains pinned to m_S for a finite range of the field strength, while in phase B the susceptibility dM/dB near zero field is finite, see Fig. 4. For sufficiently strong field, a gap opens in the minority band in phase B, too. This effect can be understood within a rigid-band picture which holds to a first approximation. For very strong field, the magnetization is reoriented in a first-order spin-flop transition which preempts another Lifshitz transition.

In Fig. 5 we plot the temperature dependence of key thermodynamic and transport properties in phases A and B. We find that the magnetization in phase B remains essentially pinned at m_S until T becomes of the order of the gap, while it has a finite temperature-derivative at $T = 0$ in phase A. This difference is, however, small. The resistance ρ increases in both phases up to the Curie temperature T_C , then it decreases approximately as a power-law $T^{-0.3}$, not logarithmically. The heat capacity c has a jump discontinuity at T_C . Similar features are indeed observed experimentally, for example in Refs. [19, 22, 23], although the simple KLM does not capture the full complexity of real materials.

We summarize the behavior of both Kondo lattice models

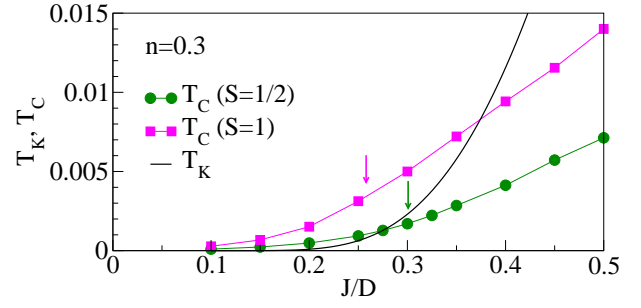


Figure 6: (Color online) “Ferromagnetic Doniach diagram” for spin-1/2 and spin-1 Kondo lattice models. The arrows indicate the position of the Lifshitz transitions.

in the form of a “ferromagnetic Doniach diagram” in Fig. 6. We plot the single-impurity Kondo temperature (which does not depend on the impurity spin [53]) and the Curie temperature T_C for each model. The Curie temperature has no observable feature at the Lifshitz transition points (indicated by the arrows) and in this parameter range it does not go to zero nor even decrease, unlike the Néel temperature in the antiferromagnetic case. These results indicate that the Kondo effect indeed favors FM ordering through the RKKY interaction [26, 33, 34]. Apart from the (approximately) factor of two difference, there is no pronounced difference in T_C of spin-1/2 and spin-1 models.

We conclude by answering the questions raised in the introduction. The ferromagnetism and local Kondo singlet formation do not compete in the same way as the antiferromagnetic ordering and the Kondo effect do; there is no Kondo breakdown and no criticality, but rather a continuous filling of the lower minority band and the disappearance of the electron pockets. We thus find robust coexistence of FM order and Kondo screening in both phases. This is the case for both spin-1/2 and spin-1 Kondo lattice models, thus the physics of Kondo underscreening does not need to be invoked to explain the magnetic ordering. Both models have qualitatively the same phase diagram in this range of filling and exchange coupling strength. The Lifshitz transitions are observable in the temperature and magnetic-field dependence of the magnetization. The static mean-field appears to be valid at the qualitative level, however to properly describe the real nature of ferromagnetic phases and transitions it is necessary to take into account dynamic effects, as in the DMFT treatment.

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- [1] P. Coleman and A. J. Schofield, *Nature* **433**, 226 (2005).
 - [2] H. Löhneysen, A. Rosch, M. Vojta, and P. Wölfle, *Reviews of Modern Physics* **79**, 1015 (2007).
 - [3] Q. Si and F. Steglich, *Science* **329**, 1161 (2010).
 - [4] G. R. Stewart, *Reviews of Modern Physics* **73**, 797 (2001).

- [5] P. Gegenwart, Q. Si, and F. Steglich, *Nature Physics* **4**, 186 (2008).
- [6] C. Pfleiderer, *Reviews of Modern Physics* **81**, 1551 (2009).
- [7] H. Tsunetsugu, M. Sigrist, and K. Ueda, *Reviews of Modern Physics* **69**, 809 (1997).
- [8] M. Gulácsi, *Advances in Physics* **53**, 769 (2004).
- [9] A. C. Hewson, *The Kondo Problem to Heavy-Fermions* (Cambridge University Press, Cambridge, 1993).
- [10] S. Doniach, *Physica B* **91**, 231 (1977).
- [11] S. Capponi and F. Assaad, *Physical Review B* **63**, 155114 (2001).
- [12] J. Otsuki, H. Kusunose, and Y. Kuramoto, *Physical Review Letters* **102**, 017202 (2009).
- [13] L. De Leo, M. Civelli, and G. Kotliar, *Physical Review Letters* **101**, 256404 (2008).
- [14] L. Martin and F. Assaad, *Physical Review Letters* **101**, 066404 (2008).
- [15] L. Martin, M. Bercx, and F. Assaad, *Physical Review B* **82**, 245105 (2010).
- [16] S. Süllow, M. C. Aronson, B. D. Rainford, and P. Haen, *Physical Review Letters* **82**, 2963 (1999).
- [17] D. Rojas, J. Espeso, J. Rodríguez Fernández, J. Gómez Sal, J. Sanchez Marcos, and H. Müller, *Physical Review B* **80**, 184413 (2009).
- [18] K. Mukherjee, K. K. Iyer, and E. V. Sampathkumaran, *Journal of Physics: Condensed Matter* **24**, 096006 (2012).
- [19] R. Baumbach, H. Chudo, H. Yasuoka, F. Ronning, E. Bauer, and J. Thompson, *Physical Review B* **85**, 094422 (2012).
- [20] J. Schoenes, B. Frick, and O. Vogt, *Physical Review B* **30**, 6578 (1984).
- [21] Z. Bukowski, R. Troć, J. Stepień-Damm, C. Sułkowski, and V. H. Tran, *Journal of Alloys and Compounds* **403**, 65 (2005).
- [22] V. Tran, R. Troć, Z. Bukowski, D. Badurski, and C. Sułkowski, *Physical Review B* **71**, 094428 (2005).
- [23] E. Colineau, F. Wastin, J. P. Sanchez, and J. Rebizant, *Journal of Physics: Condensed Matter* **20**, 075207 (2008).
- [24] V. Tran, J. C. Griveau, R. Eloirdi, W. Miiller, and E. Colineau, *Physical Review B* **82**, 094407 (2010).
- [25] R. Troć, M. Samsel-Czekala, J. Stepień-Damm, and B. Coqblin, *Physical Review B* **85**, 224434 (2012).
- [26] N. B. Perkins, J. R. Iglesias, M. D. Núñez-Regueiro, and B. Coqblin, *Europhysics Letters (EPL)* **79**, 57006 (2007).
- [27] N. Perkins, M. Núñez Regueiro, B. Coqblin, and J. Iglesias, *Physical Review B* **76**, 125101 (2007).
- [28] B. Coqblin, J. R. Iglesias, N. B. Perkins, A. S. d. R. Simoes, and C. Thomas, *Physica B: Condensed Matter* **404**, 2961 (2009).
- [29] C. Thomas, A. da Rosa Simões, J. Iglesias, C. Lacroix, N. Perkins, and B. Coqblin, *Physical Review B* **83**, 014415 (2011).
- [30] C. Lacroix and M. Cyrot, *Physical Review B* **20**, 1969 (1979).
- [31] C. Batista, J. Bonča, and J. Gubernatis, *Physical Review Letters* **88**, 187203 (2002).
- [32] R. Peters and T. Pruschke, *Phys. Rev. B* **76**, 245101 (2007).
- [33] J. Otsuki, H. Kusunose, and Y. Kuramoto, *J. Phys. Soc. Japan* **78**, 034719 (2009).
- [34] R. Peters, N. Kawakami, and T. Pruschke, *Phys. Rev. Lett.* **108**, 086402 (2012).
- [35] M. Katsnelson, V. Irkhin, L. Chioncel, A. Lichtenstein, and R. de Groot, *Reviews of Modern Physics* **80**, 315 (2008).
- [36] K. S. D. Beach and F. F. Assaad, *Phys. Rev. B* **77**, 205123 (2008).
- [37] S. Viola Kusminskiy, K. Beach, A. Castro Neto, and D. Campbell, *Physical Review B* **77**, 094419 (2008).
- [38] Y. Liu, G.-M. Zhang, and L. Yu, *Weak ferromagnetism induced by the Kondo screening effect in the Kondo lattice systems*, cond-mat:1301.1771 (2013).
- [39] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, *Rev. Mod. Phys.* **68**, 13 (1996).
- [40] K. G. Wilson, *Rev. Mod. Phys.* **47**, 773 (1975).
- [41] R. Bulla, T. Costi, and T. Pruschke, *Rev. Mod. Phys.* **80**, 395 (2008).
- [42] W. Hofstetter, *Phys. Rev. Lett.* **85**, 1508 (2000).
- [43] R. Peters, T. Pruschke, and F. B. Anders, *Phys. Rev. B* **74**, 245114 (2006).
- [44] A. Weichselbaum and J. von Delft, *Phys. Rev. Lett.* **99**, 076402 (2007).
- [45] R. Žitko and T. Pruschke, *Phys. Rev. B* **79**, 085106 (2009).
- [46] T. Pruschke, R. Bulla, and M. Jarrell, *Phys. Rev. B* **61**, 12799 (2000).
- [47] T. A. Costi and N. Manini, *J. Low. Temp. Phys.* **126**, 835 (2002).
- [48] I. M. Lifshitz, *Sov. Phys. JEPT* **11**, 1130 (1960).
- [49] Y. Yamaji, T. Misawa, and M. Imada, *Journal of the Physical Society of Japan* **75**, 094719 (2006).
- [50] G.-B. Li, G.-M. Zhang, and Y. Lu, *Physical Review B* **81**, 094420 (2010).
- [51] M. Bercx and F. F. Assaad, *Phys. Rev. B* **86**, 075108 (2012).
- [52] R. Peters, Private communication.
- [53] N. Andrei, K. Furuya, and J. H. Lowenstein, *Rev. Mod. Phys.* **55**, 331 (1983).